Deep learning in drug discovery: an integrative review and future challenges

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Abstract

Recently, using artificial intelligence (AI) in drug discovery has received much attention since it significantly shortens the time and cost of developing new drugs. Deep learning (DL)-based approaches are increasingly being used in all stages of drug development as DL technology advances, and drug-related data grows. Therefore, this paper presents a systematic Literature review (SLR) that integrates the recent DL technologies and applications in drug discovery Including, drug–target interactions (DTIs), drug–drug similarity interactions (DDIs), drug sensitivity and responsiveness, and drug-side effect predictions. We present a review of more than 300 articles between 2000 and 2022. The benchmark data sets, the databases, and the evaluation measures are also presented. In addition, this paper provides an overview of how explainable AI (XAI) supports drug discovery problems. The drug dosing optimization and success stories are discussed as well. Finally, digital twining (DT) and open issues are suggested as future research challenges for drug discovery problems. Challenges to be addressed, future research directions are identified, and an extensive bibliography is also included.